STN Search History

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Connecting via Winsock to STN


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TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page for STN Seminar Schedule - N. America
 NEWS  2  MAY 01   New CAS web site launched
 NEWS  3  MAY 08   CA/CAplus Indian patent publication number format defined
 NEWS  4  MAY 14   RDISCLOSURE on STN Easy enhanced with new search and display
                   fields
 NEWS  5  MAY 21   BIOSIS reloaded and enhanced with archival data
 NEWS  6  MAY 21   TOXCENTER enhanced with BIOSIS reload
 NEWS  7  MAY 21   CA/CAplus enhanced with additional kind codes for German
                   patents
 NEWS  8  MAY 22   CA/CAplus enhanced with IPC reclassification in Japanese
                   patents
 NEWS  9  JUN 27   CA/CAplus enhanced with pre-1967 CAS Registry Numbers
 NEWS 10  JUN 29   STN Viewer now available
 NEWS 11  JUN 29   STN Express, Version 8.2, now available
 NEWS 12  JUL 02   LEMBASE coverage updated
 NEWS 13  JUL 02   LMEDLINE coverage updated
 NEWS 14  JUL 02   SCISEARCH enhanced with complete author names
 NEWS 15  JUL 02   CHEMCATS accession numbers revised
 NEWS 16  JUL 02   CA/CAplus enhanced with utility model patents from China
 NEWS 17  JUL 16   CAplus enhanced with French and German abstracts
 NEWS 18  JUL 18   CA/CAplus patent coverage enhanced
 NEWS 19  JUL 26   USPATFULL/USPAT2 enhanced with IPC reclassification
 NEWS 20  JUL 30   USGENE now available on STN
 NEWS 21  AUG 06   CAS REGISTRY enhanced with new experimental property tags
 NEWS 22  AUG 06   BEILSTEIN updated with new compounds
 NEWS 23  AUG 06   FSTA enhanced with new thesaurus edition
 NEWS 24  AUG 13   CA/CAplus enhanced with additional kind codes for granted
                   patents
 NEWS 25  AUG 20   CA/CAplus enhanced with CAS indexing in pre-1907 records
 NEWS 26  AUG 27   Full-text patent databases enhanced with predefined
                   patent family display formats from INPADOCDB
 NEWS 27  AUG 27   USPATOLD now available on STN
 NEWS 28  AUG 28   CAS REGISTRY enhanced with additional experimental
                   spectral property data

 NEWS EXPRESS  29 JUNE 2007:  CURRENT WINDOWS VERSION IS V8.2,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8
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Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:51:23 ON 28 AUG 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:51:30 ON 28 AUG 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 AUG 2007 HIGHEST RN 945649-99-0
DICTIONARY FILE UPDATES: 27 AUG 2007 HIGHEST RN 945649-99-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

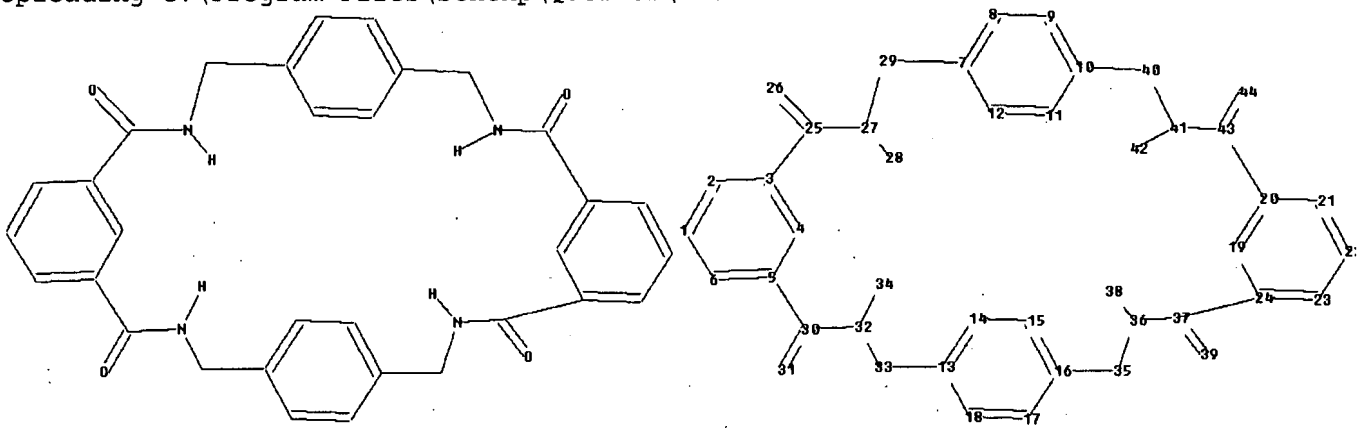
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10597663.str



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ring nodes :
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24 25 27 29 30 32 33 35 36 37 40 41 43
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25-26 27-28 30-31 32-34 36-38 37-39 41-42 43-44
ring bonds :
1-2 1-6 2-3 3-4 3-25 4-5 5-6 5-30 7-8 7-12 7-29 8-9 9-10 10-11 10-40
11-12 13-14 13-18 13-33 14-15 15-16 16-17 16-35 17-18 19-20 19-24 20-21
20-43 21-22 22-23 23-24 24-37 25-27 27-29 30-32 32-33 35-36 36-37 40-41
41-43
exact/norm bonds :
3-25 5-30 7-29 10-40 13-33 16-35 20-43 24-37 25-26 25-27 27-29 30-31
30-32 32-33 35-36 36-37 37-39 40-41 41-43 43-44
exact bonds :
27-28 32-34 36-38 41-42
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-
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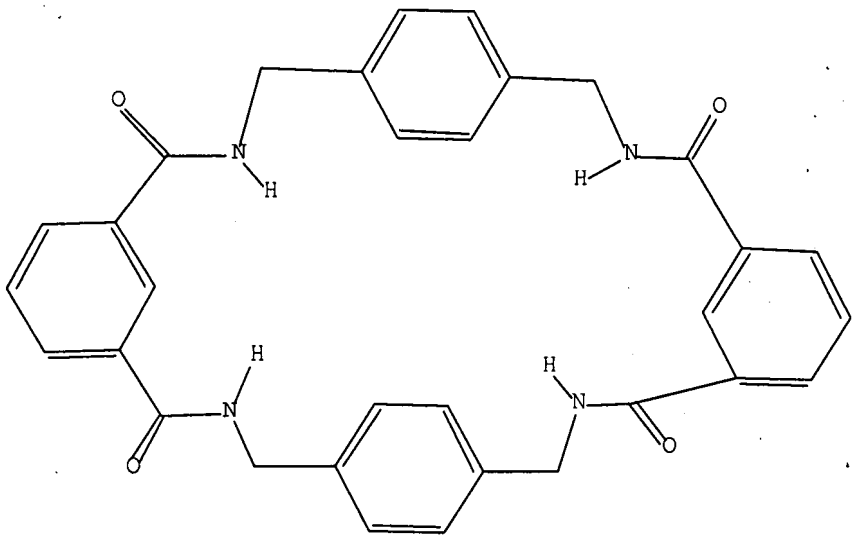
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:Atom 28:CLASS
29:Atom 30:Atom 31:CLASS 32:Atom 33:Atom 34:CLASS 35:Atom 36:Atom 37:Atom
38:CLASS 39:CLASS 40:Atom 41:Atom 42:CLASS 43:Atom 44:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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=> s l1
SAMPLE SEARCH INITIATED 15:52:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     1231 TO ITERATE

100.0% PROCESSED     1231 ITERATIONS                                 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        22516 TO    26724
PROJECTED ANSWERS:               9 TO      360

L2             9 SEA SSS SAM L1

=> d scan

L2    9 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN    Glycine, N-(diphenylacetyl)glycyl-, [[(4-methylphenyl)sulfonyl]sulfinimido
      yl]di-3,1-propanediyl ester, rotaxane compd. with 3,11,18,26-
      tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-
      5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone
      (1:1) (9CI)
MF    C49 H53 N5 O10 S2 . C32 H28 N4 O4

      CM   1
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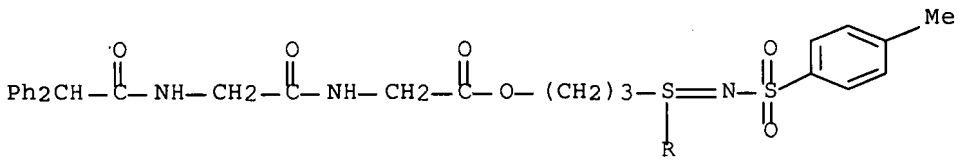

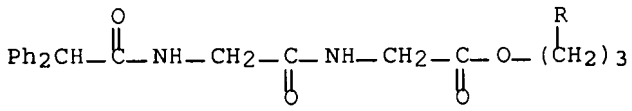


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      CM   2
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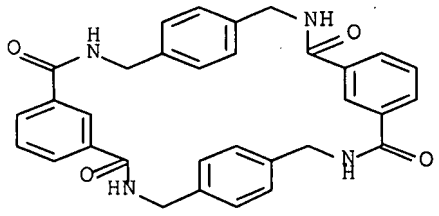


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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1
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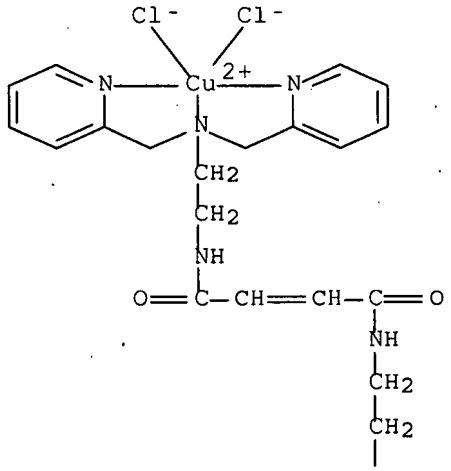
L2 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Copper, [μ-[N,N'-bis[2-[bis[(2-pyridinyl-κN)methyl]amino-κN]ethyl]-2-butenediamide]]tetrachlorodi-, rotaxane compd. with N,N-dimethylformamide and 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:2:1) (9CI)

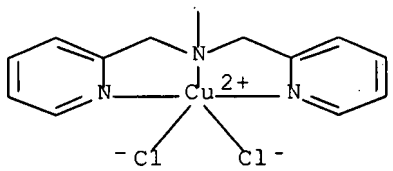
MF C32 H36 Cl4 Cu2 N8 O2 . C32 H28 N4 O4 . 2 C3 H7 N O

CM 1

PAGE 1-A



PAGE 2-A



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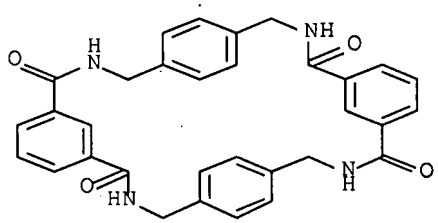

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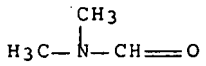
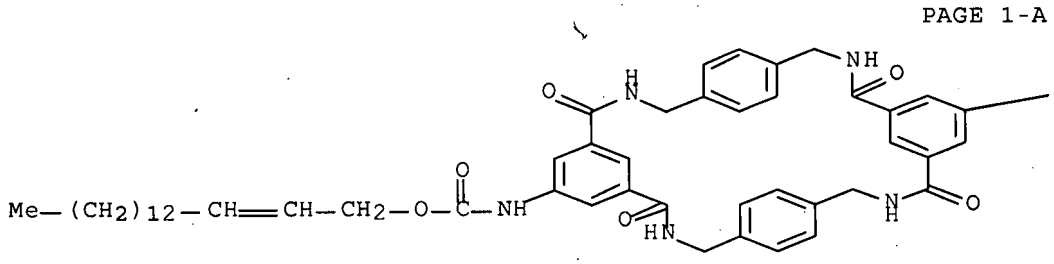


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Carbamic acid, [22-(1,1-dimethylethyl)-4,10,19,25-tetraoxo-3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(34),13,15,20,22,24(33),28,30,31,35-dodecaen-7-yl]-, 2-hexadecenyl ester (9CI)
MF C53 H67 N5 O6
CI COM

PAGE 1-A



PAGE 1-B

Bu-t

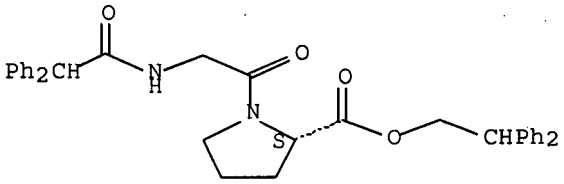
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

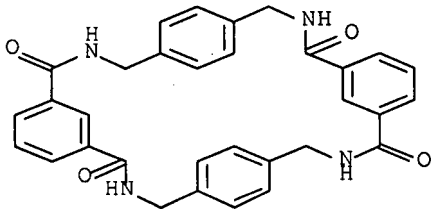
L2 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN L-Proline, N-(diphenylacetyl)glycyl-, 2,2-diphenylethyl ester, rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (9CI)
MF C35 H34 N2 O4 . C32 H28 N4 O4

CM 1

Absolute stereochemistry.



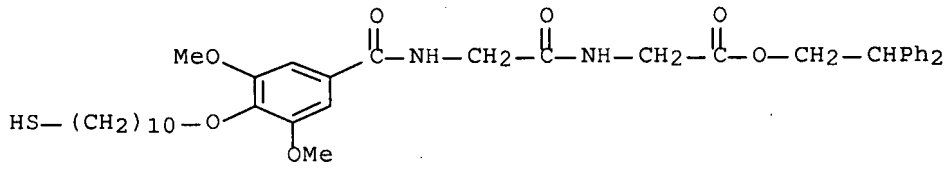
CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Glycine, N-[4-[(10-mercaptodecyl)oxy]-3,5-dimethoxybenzoyl]glycyl-, 2,2-diphenylethyl ester, rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (9CI)
MF C37 H48 N2 O7 S . C32 H28 N4 O4

CM 1



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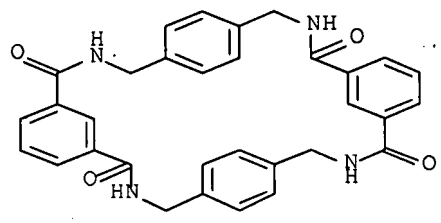
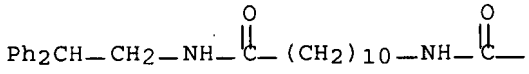


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Butanediamide, N-[11-[(2,2-diphenylethyl)amino]-11-oxoundecyl]-N'-[2-(2'H-[5,6]fullereno-C60-Ih-[1,9-c]pyrrol-1'(5'H)-yl)ethyl]-, radical ion(1-), rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1)
MF C93 H48 N4 O3 . C32 H28 N4 O4

CM 1

PAGE 1-A



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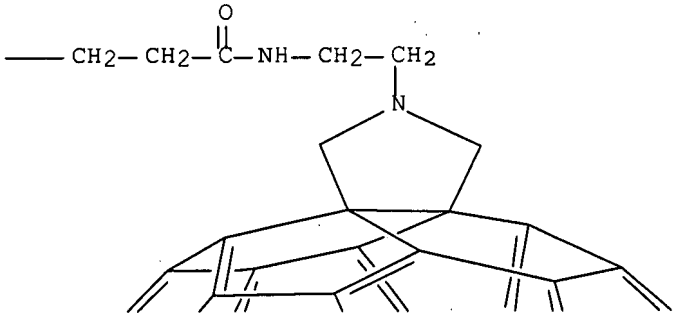

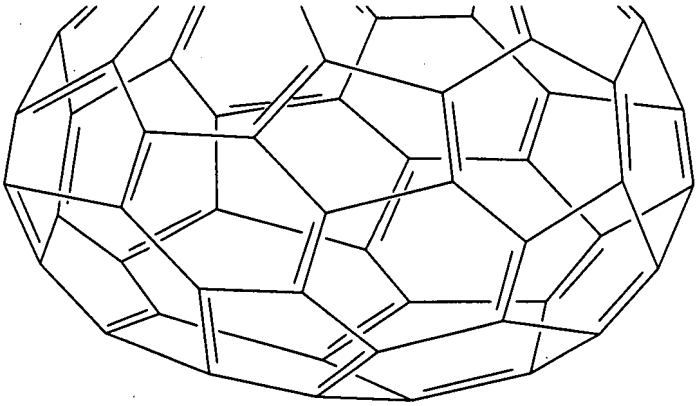

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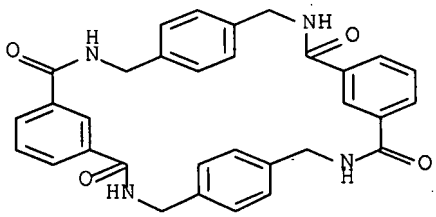
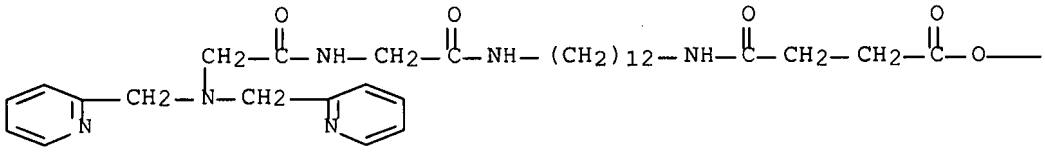


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

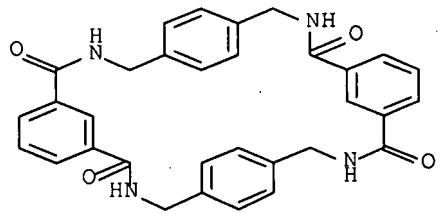
L2 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Glycinamide, N,N-bis(2-pyridinylmethyl)glycyl-N-[12-[[4-(2,2-diphenylethoxy)-1,4-dioxobutyl]amino]dodecyl]-, rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (9CI)
MF C46 H60 N6 O5 . C32 H28 N4 O4

CM 1



—CH2—CHPh2

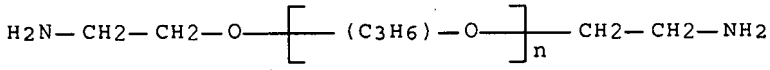
CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Butenediamide, N,N,N',N'-tetrakis[6-[[(hexahydro-2-oxo-1H-azepin-1-yl)carbonyl]amino]hexyl]-, (2E)-, rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1), polymer with α-(2-aminomethylethyl)-ω-(2-aminomethylethoxy)poly[oxy(methyl-1,2-ethanediyl)] (9CI)
MF (C56 H94 N10 O10 . C32 H28 N4 O4 . (C3 H6 O)n C6 H16 N2 O)x
CI PMS

CM 1



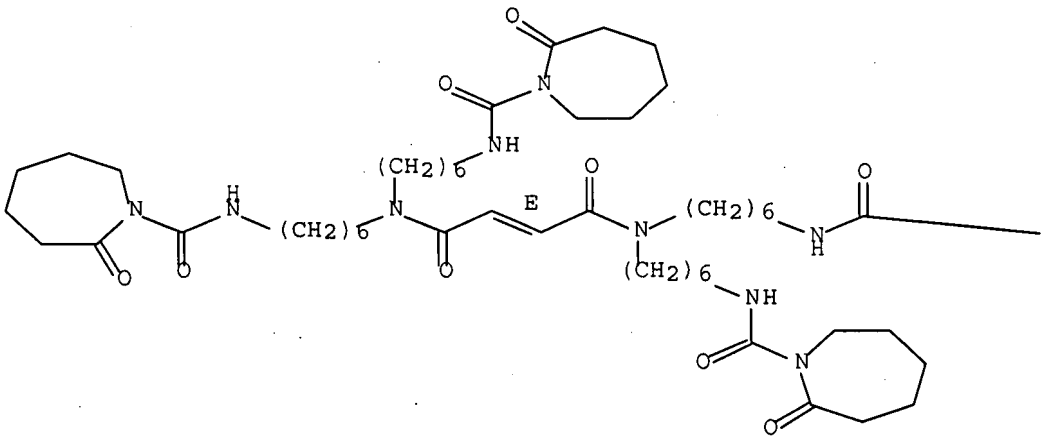
2 (D1—Me)

CM 2

CM 3

Double bond geometry as shown.

PAGE 1-A



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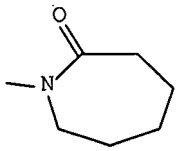

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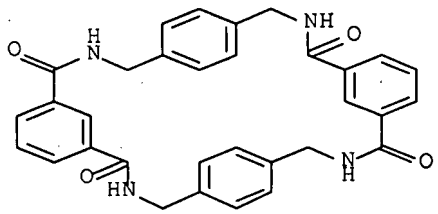


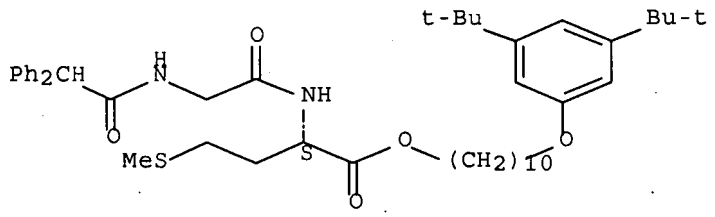
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN L-Methionine, N-(diphenylacetyl)glycyl-, 10-[3,5-bis(1,1-dimethylethyl)phenoxy]decyl ester, rotaxane compd. with 7,22-bis(2-propenyloxy)-3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (9CI)

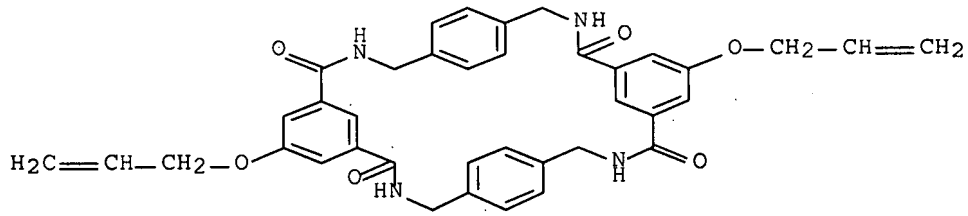
MF C45 H64 N2 O5 S . C38 H36 N4 O6

CM 1

Absolute stereochemistry.



CM 2



ALL ANSWERS HAVE BEEN SCANNED

=> 1

FILE 'CAPLUS' ENTERED AT 15:57:13 ON 28 AUG 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 28 Aug 2007 VOL 147 ISS 10
FILE LAST UPDATED: 27 Aug 2007 (20070827/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=>

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 8 ANSWERS - CONTINUE? Y/(N):y

L6 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1042566 CAPLUS Full-text
DOCUMENT NUMBER: 146:7581
TITLE: Reverse Shuttling in a Fullerene-Stoppered Rotaxane
AUTHOR(S): Mateo-Alonso, Aurelio; Fioravanti, Giulia; Marcaccio, Massimo; Paolucci, Francesco; Jagesar, Dhiredj C.; Brouwer, Albert M.; Prato, Maurizio
CORPORATE SOURCE: INSTM unit of Trieste and Dipartimento di Scienze Farmaceutiche, Universita degli Studi di Trieste, Trieste, 34127, Italy
SOURCE: Organic Letters (2006), 8(22), 5173-5176
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:7581

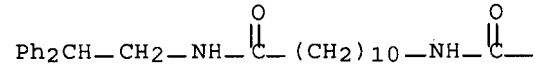
AB The prepn. and characterization of a solvent-switchable rotaxane that shuttles in the opposite direction to that expected are reported. The reverse shuttling is confirmed by NMR spectroscopy and can be monitored by cyclic voltammetry. The electrochem. generated anions on the fullerene moiety are stabilized by the closer proximity of the macrocycle.

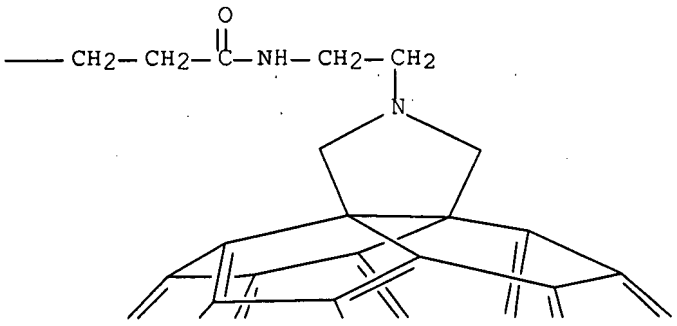
IT 913943-50-7
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(reverse shuttling in fullerene-stoppered rotaxane)

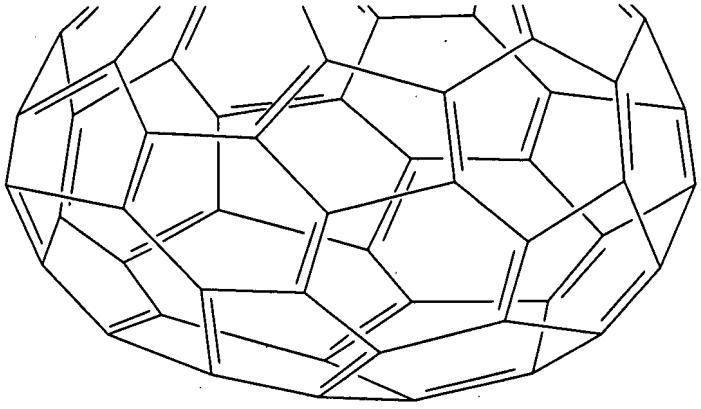
RN 913943-50-7 CAPLUS
CN Butanediamide, N-[11-[(2,2-diphenylethyl)amino]-11-oxoundecyl]-N'-[2-(2'H-[5,6]fullereno-C60-Ih-[1,9-c]pyrrol-1'(5'H)-yl)ethyl]-, radical ion(1-), rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (CA INDEX NAME)

CM 1

CRN 913943-49-4
CMF C93 H48 N4 O3
CCI RIS

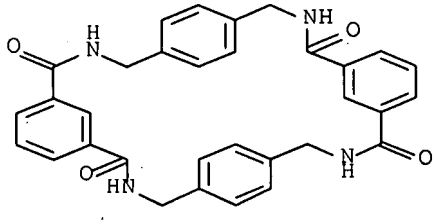






CM 2

CRN 169203-75-2
CMF C32 H28 N4 O4



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:219952 CAPLUS Full-text
DOCUMENT NUMBER: 144:444544
TITLE: An allosterically regulated molecular shuttle
AUTHOR(S): Marlin, Dana S.; Cabrera, Diego Gonzalez; Leigh, David A.; Slawin, Alexandra M. Z.
CORPORATE SOURCE: School of Chemistry, University of Edinburgh, Edinburgh, EH9 3JJ, UK
SOURCE: Angewandte Chemie, International Edition (2006), 45(9), 1385-1390
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:444544

AB A switchable rotaxane was developed in which the binding of a metal ion (e.g. Cd2+) to a bis(picolyl)amine fragment that acts as one of the stoppers induces a shift of the macrocyclic component along the thread from one binding site to another weaker binding site. Crystal structures were determined for two metal-free rotaxanes and for three copper complexes.

IT 884592-09-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of copper complex of a rotaxane with thread having dipicolylamine chelating group)

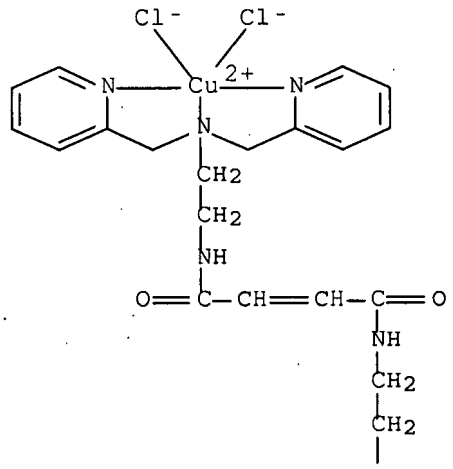
RN 884592-09-0 CAPLUS

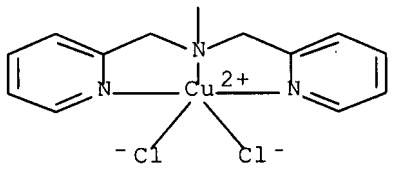
CN Copper, [μ-[N,N'-bis[2-[bis[(2-pyridinyl-κN)methyl]amino-κN]ethyl]-2-butenediamide]]tetrachlorodi-, rotaxane compd. with N,N-dimethylformamide and 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 884592-08-9
CMF C32 H36 Cl4 Cu2 N8 O2
CCI CCS

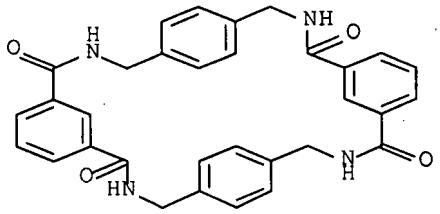
PAGE 1-A





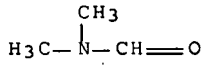
CM 2

CRN 169203-75-2
CMF C32 H28 N4 O4



CM 3

CRN 68-12-2
CMF C3 H7 N O



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:17634 CAPLUS Full-text
DOCUMENT NUMBER: 144:245942
TITLE: Complexation-induced translational isomerism: Shuttling through stepwise competitive binding
AUTHOR(S): Marlin, Dana S.; Cabrera, Diego Gonzalez; Leigh, David A.; Slawin, Alexandra M. Z.
CORPORATE SOURCE: School of Chemistry, University of Edinburgh, Edinburgh, EH93JJ, UK
SOURCE: Angewandte Chemie, International Edition (2006), 45(1), 77-83
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:245942

AB Progressive binding of a transition-metal ion to a peptide station displaces the macrocycle to an alternative station in a H-bonded mol. shuttle. Cu(HL)Cl2 (HL = 5-((RCH2)2NCH2CONH)C6H3(CO2Me)2-1,3 (R = 2-pyridyl)), was prepared and reacted with CuCl2 or NaH to give [Cu(HL)Cl]2[CuCl4] and CuLCl, resp. (RCH2)2NCH2CONHCH2CONHCH2CHPh2 (H2L1) reacted with Cu and Cd salts to give Cu(H2L1)Cl2 and Cd(H2L1)(NO3)2 which were deprotonated to give Cu(HL1)Cl and Cd(HL1)(NO3), resp., with change in the coordination environment. The rotaxane H2L1.L2 (L = 2,6,15,19-tetraoxo-1,7,14,20-tetraaza-3,5,9,12,16,18,22,25- tetrabenzocyclohexancosane), prepared from p-xylylenediamine and isophthaloyl chloride, was prepared and reacted with Cu and Cd salts to give Cu(H2L1.L2)Cl2 and Cd(H2L1.L2)(NO3)2, resp. Deprotonation of Cu(H2L1.L2)Cl2 gave Cu(HL1.L2)Cl with change in the coordination environment and subsequently with degradation of the rotaxane structure. The rotaxane H2L3.L2 (H2L3 = (RCH2)2NCH2CONHCH2CONH(CH2)12NHCOCH2CH2CO2CH2CHPh 2) reacted with Cu and Cd salts to give Cu(H2L3.L2)Cl2 and Cd(H2L3.L2)(NO3)2 which were deprotonated to give Cu(HL3.L2)Cl and Cd(HL3.L2)(NO3), resp., with shuttling of L2 to an alternative station in the H-bonded mol. shuttle. The crystal structures of several of these complexes were determined

IT 876289-70-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(rotaxane; preparation and complexation with cadmium and copper)

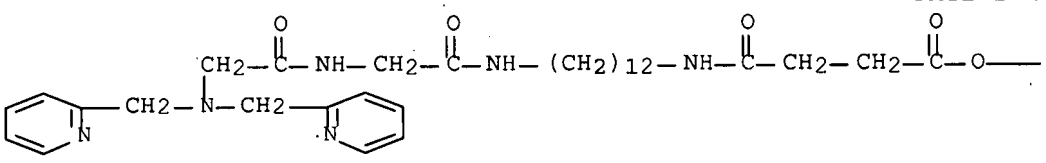
RN 876289-70-2 CAPLUS

CN Glycinamide, N,N-bis(2-pyridinylmethyl)glycyl-N-[12-[[4-(2,2-diphenylethoxy)-1,4-dioxobutyl]amino]dodecyl]-, rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 876289-69-9
CMF C46 H60 N6 O5

PAGE 1-A

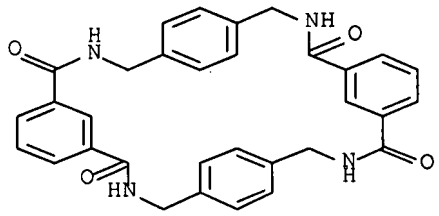


PAGE 1-B

—CH2—CHPh2

CM 2

CRN 169203-75-2
CMF C32 H28 N4 O4



REFERENCE COUNT: 98 THERE ARE 98 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:638951 CAPLUS Full-text
DOCUMENT NUMBER: 139:292587
TITLE: Rotaxane building blocks bearing blocked isocyanate stoppers: Polyrotaxanes through post-assembly chain extension
AUTHOR(S): Kidd, Timothy J.; Loontjens, Ton J. A.; Leigh, David A.; Wong, Jenny K. Y.
CORPORATE SOURCE: DSM Research, Geleen, 6160 MD, Neth.
SOURCE: Angewandte Chemie, International Edition (2003), 42(29), 3379-3383
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

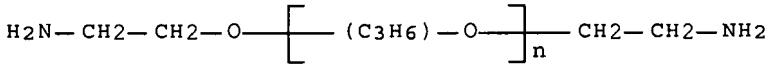
AB A simple, versatile route to polyamide-polyoxyalkylene-polyurea polyrotaxanes with a variety of topologies is available through the synthesis and subsequent polymerization of readily accessible, stable, rotaxane monomers containing bulky, blocked isocyanate stopper groups. These monomeric [2]rotaxanes represent a new kind of functional-chain extender that is wholly compatible with methodologies currently used to make a range of com. polymers and could thus lead to the facile incorporation of a number of rotaxane systems into materials where the effects of the mech. bond could be tested and realistically exploited. In principle, this system can also be applied to the modular generation of rotaxane-based polymeric materials or devices in which individual components can be introduced in different combinations through "bottom-up" processing.

IT **609842-48-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(rotaxane building blocks bearing blocked isocyanate stoppers used to prepare polyrotaxanes through post-assembly chain extension)

RN 609842-48-0 CAPLUS
CN 2-Butenediamide, N,N,N',N'-tetrakis[6-[[(hexahydro-2-oxo-1H-azepin-1-yl)carbonyl]amino]hexyl]-, (2E)-, rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1), polymer with α-(2-aminomethylethyl)-ω-(2-aminomethylethoxy)poly[oxy(methyl-1,2-ethanediyl)] (9CI) (CA INDEX NAME)

CM 1

CRN 9046-10-0
CMF (C3 H6 O)n C6 H16 N2 O
CCI IDS, PMS



2 (D1—Me)

CM 2

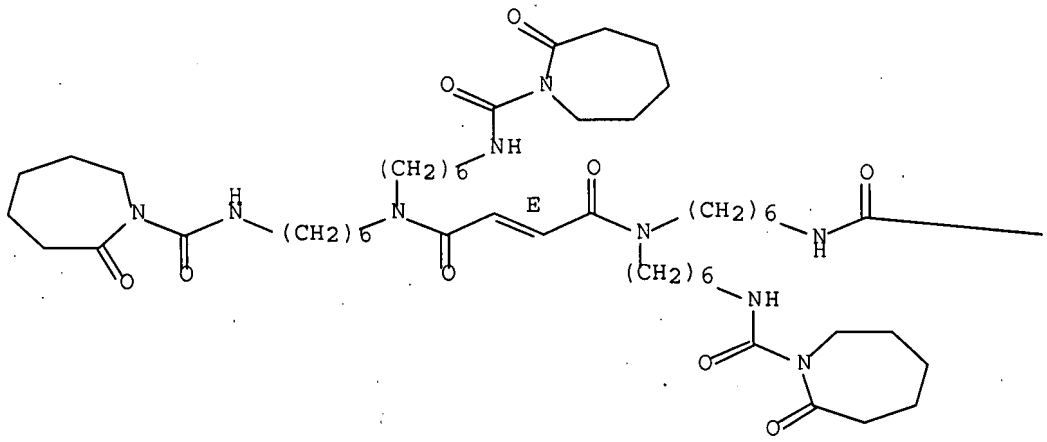
CRN 609842-43-5
CMF C56 H94 N10 O10 . C32 H28 N4 O4

CM 3

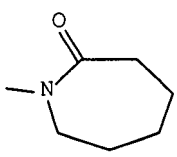
CRN 609842-42-4
CMF C56 H94 N10 O10

Double bond geometry as shown.

PAGE 1-A

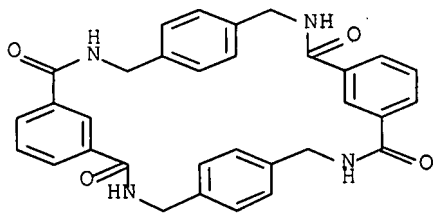


PAGE 1-B



CM 4

CRN 169203-75-2
CMF C32 H28 N4 O4



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:159908 CAPLUS Full-text
DOCUMENT NUMBER: 136:340989
TITLE: Switching "On" and "Off" the Expression of Chirality in Peptide Rotaxanes
AUTHOR(S): Asakawa, Masumi; Brancato, Giuseppe; Fanti, Marianna; Leigh, David A.; Shimizu, Toshimi; Slawin, Alexandra M. Z.; Wong, Jenny K. Y.; Zerbetto, Francesco; Zhang, Songwei
CORPORATE SOURCE: Nanoarchitectonics Research Center, National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, 305-8565, Japan
SOURCE: Journal of the American Chemical Society (2002), 124(12), 2939-2950
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:340989

AB The hydrogen-bond-directed synthesis, x-ray crystal structures, and optical properties of the first chiral peptide rotaxanes are reported. Collectively these systems provide the first examples of single mol. species where the expression of chirality in the form of a CD response can selectively be switched "on" or "off", and its magnitude altered, through controlling the interactions between mech. interlocked submol. components. The switching is achievable both thermally and through changes in the nature of the environment. Peptido[2]rotaxanes consisting of an intrinsically achiral benzylic amide macrocycle locked onto various chiral dipeptide (Gly-Ala, Gly-Leu, Gly-Met, Gly-Phe, and Gly-Pro) threads exhibit strong (10-20k deg cm2 dmol-1) neg. induced CD (θ) values in nonpolar solvents (e.g. CHCl3), where the intramol. hydrogen bonding between thread and macrocycle is maximized. In polar solvents (e.g., MeOH), where the intercomponent hydrogen bonding is weakened, or switched off completely, the elliptical polarization falls close to zero in some cases and can even be switched to large pos. values in others. Importantly, the mechanism of generating the switchable CD response in the chiral peptide rotaxanes is also determined: a combination of semiempirical calcns. and geometrical modeling using the continuous chirality measure (CCM) shows that the chirality is transmitted from the amino acid asym. center on the thread via the macrocycle to the C-terminal stopper of the rotaxane. This

understanding could have important implications for other areas where chiral transmission from one chemical entity to another underpins a phys. or chemical response, such as the seeding of supertwisted nematic liquid crystalline phases or asym. synthesis.

IT 419537-14-7P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation, crystal structures and optical properties of peptide rotaxanes
to study the switching "on" and "off" their expression of chirality)

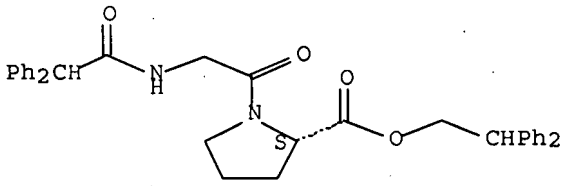
RN 419537-14-7 CAPLUS

CN L-Proline, N-(diphenylacetyl)glycyl-, 2,2-diphenylethyl ester, rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (9CI) (CA INDEX NAME)

CM 1

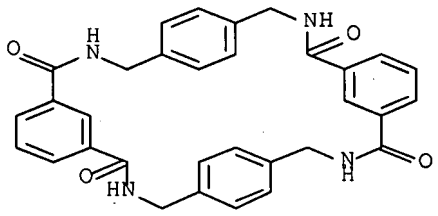
CRN 419537-13-6
CMF C35 H34 N2 O4

Absolute stereochemistry.



CM 2

CRN 169203-75-2
CMF C32 H28 N4 O4



REFERENCE COUNT: 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

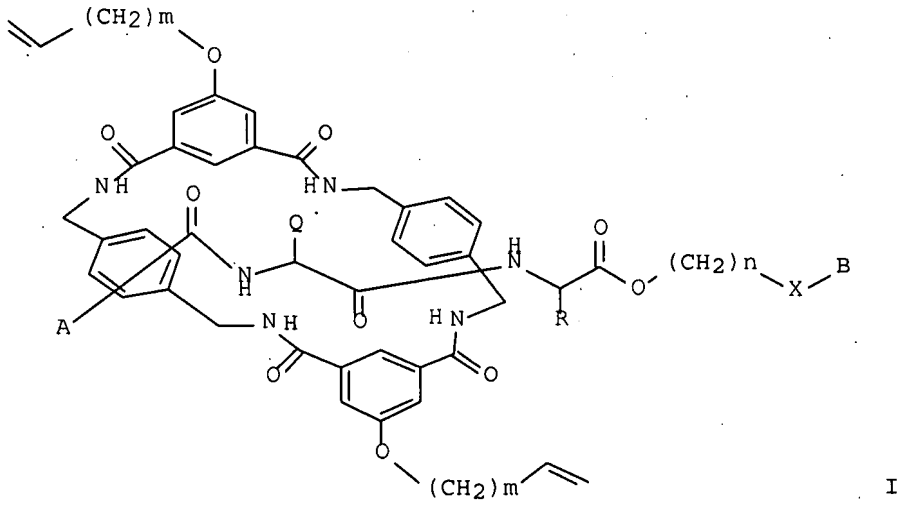
L6 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:21352 CAPLUS Full-text
DOCUMENT NUMBER: 134:72032
TITLE: Intermediates for manufacture of polymers containing rotaxanes having a cyclotetraamide ring in main chains
INVENTOR(S): Asakawa, Masumi; Murphy, Aden; Leigh, David A.;

	Shimizu, Toshimi
PATENT ASSIGNEE(S):	Agency of Industrial Sciences and Technology, Japan; National Institute of Advanced Industrial Science and Technology
SOURCE:	Jpn. Kokai Tokkyo Koho, 15 pp. CODEN: JKXXAF
DOCUMENT TYPE:	Patent
LANGUAGE:	Japanese
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001002663	A	20010109	JP 1999-176952	19990623
JP 3550646	B2	20040804		
PRIORITY APPLN. INFO.:			JP 1999-176952	19990623
OTHER SOURCE(S):	MARPAT 134:72032			

GI



I

AB The intermediates are rotaxanes of I type compds. (A, B = arom. hydrocarbyl; Q, R = H, C1-5 aliphatic hydrocarbyl, aromatic hydrocarbyl, hydrocarbyl sulfide; X = CH2, O, S, CO, COO, OCO or CONH; n = 2-18; m = 1-5) which can be used as intermediates or monomers for polymers. Thus, heating 3.1 g diphenylacetylglycylglycine Et ester with 3.6 g 10-(3,5-di-tert-butylphenoxy)decan-1-ol in the presence of Sn catalyst in PhMe gave a dumb bell-like compound, 1.0 g of which was reacted with 3.1 g 5-allyloxyisophthalic acid dichloride and 1.6 g p-xylenediamine in CHCl3 to give a rotaxane at 40% yield.

IT **315199-49-6P**

RL: IMF (Industrial manufacture); PREP (Preparation)
(intermediates for manufacture of polymers containing rotaxanes having a cyclotetraamide ring in main chains)

RN 315199-49-6 CAPLUS

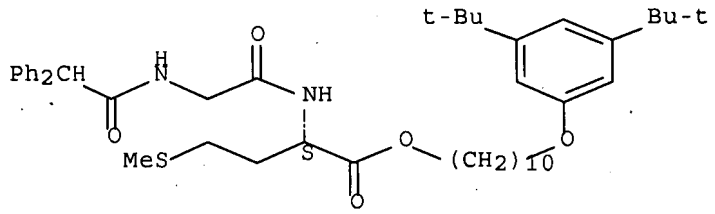
CN L-Methionine, N-(diphenylacetyl)glycyl-, 10-[3,5-bis(1,1-dimethylethyl)phenoxy]decyl ester, rotaxane compd. with 7,22-bis(2-propenyloxy)-3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.1

20,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (9CI) (CA INDEX NAME)

CM 1

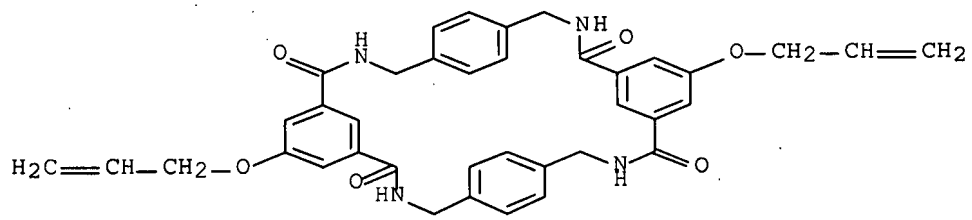
CRN 315199-37-2
CMF C45 H64 N2 O5 S

Absolute stereochemistry.



CM 2

CRN 169203-96-7
CMF C38 H36 N4 O6



L6 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:363906 CAPLUS Full-text
DOCUMENT NUMBER: 133:79887
TITLE: Self-assembly of mechanically interlocked and threaded rings. A HREELS and XPS study of thiol-functionalized catenane and rotaxane molecules on Au(111)
AUTHOR(S): De Nadai, C.; Whelan, C. M.; Perollier, C.; Clarkson, G.; Leigh, D. A.; Caudano, R.; Rudolf, P.
CORPORATE SOURCE: Laboratoire Interdisciplinaire de Spectroscopie Electronique, Facultes Universitaires Notre-Dame de la Paix, Namur, B-5000, Belg.
SOURCE: Surface Science (2000), 454-456, 112-117
CODEN: SUSCAS; ISSN: 0039-6028
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Thiol-functionalized catenane and rotaxane thin films were investigated to understand the self-assembly of such complex mols. on Au(111). Adsorption from the liquid phase at 300 K leads to the formation of overlayers without long-range order, as evidenced by high-resolution electron energy-loss spectroscopy (HREELS). As expected for thiol adsorption, the S 2p binding

energies determined by XPS are consistent with the formation of thiolate surface intermediates. The properties of these films are explored as a function of annealing. Changes in vibrational spectra such as the emergence of a Au-O band and variations in core-level binding energies and intensities reveal mol. rearrangement due to partial desorption. In addition, based on coherent domain sizes estimated by the angular width of the elastic beam intensity, annealing promotes long-range order within the adlayers.

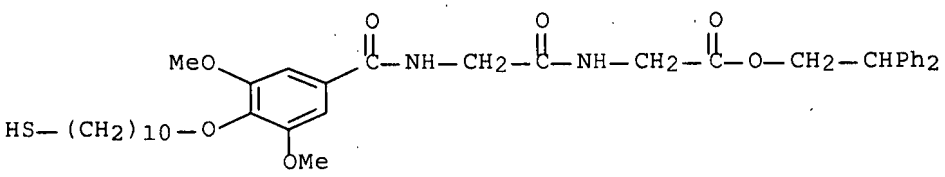
IT 280129-95-5
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(rotaxane; self-assembly of mech. interlocked and threaded rings of thiol-functionalized catenane and rotaxane mols. on Au(111) studied by HREELS and XPS)

RN 280129-95-5 CAPLUS

CN Glycine, N-[4-[(10-mercaptodecyl)oxy]-3,5-dimethoxybenzoyl]glycyl-, 2,2-diphenylethyl ester, rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (9CI) (CA INDEX NAME)

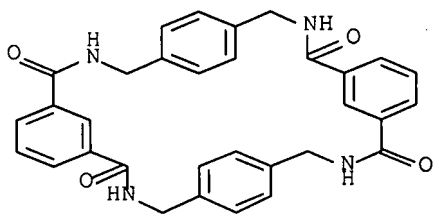
CM 1

CRN 280129-94-4
CMF C37 H48 N2 O7 S



CM 2

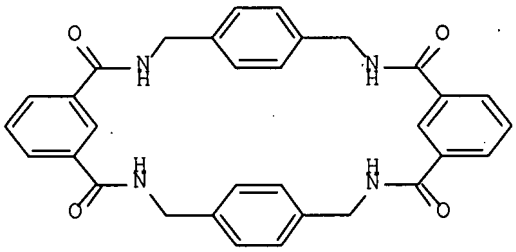
CRN 169203-75-2
CMF C32 H28 N4 O4



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:727264 CAPLUS Full-text
DOCUMENT NUMBER: 127:293615
TITLE: Peptide-Based Molecular Shuttles

AUTHOR(S): Lane, Alexander S.; Leigh, David A.; Murphy, Aden
CORPORATE SOURCE: Department of Chemistry, University of Manchester Institute of Science and Technology, Manchester, M60 1QD, UK
SOURCE: Journal of the American Chemical Society (1997), 119(45), 11092-11093
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Peptide-based mol. shuttles, composed of macrocycle I threaded on glycylglycine chains [Ph2CHCO-Gly-Gly-O(CH2)3]2X [X = CH2CH2, (CH2)10, S], were prepared and their solvent-dependent translational isomerism studied by 1H NMR. Calcns. based on variable temperature 1H NMR data give a ΔG.thermod. for shuttling in halogenated solvents (CDCl3, CD2Cl2) of 11.2, 12.4, and and 10.9 ± 0.3 kcal mol-1, resp., for I, which correspond to shuttling rates of 37,000, 5200, and 62,000 s-1, resp., at 298K. Chemical derivatization of I (X = S) to the corresponding sulfoxide or sulfone has no effect on the rate of shuttling, but the shuttling can be stopped by introduction of a bulky tosylimino group.

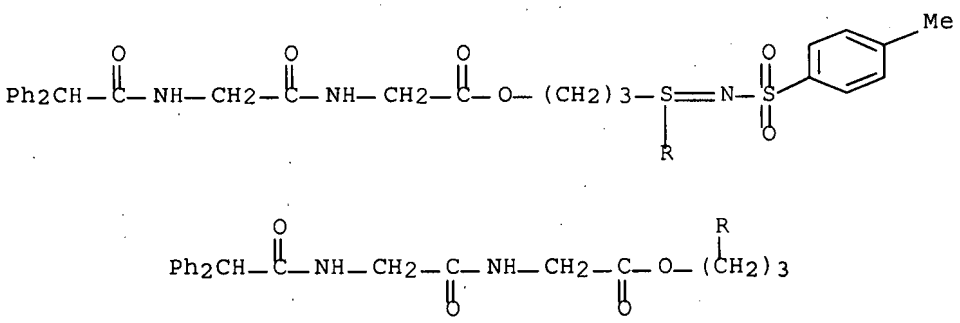
IT 196867-86-4P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and positional isomerization of peptide-based rotaxane mol. shuttles)

RN 196867-86-4 CAPLUS

CN Glycine, N-(diphenylacetyl)glycyl-, [[(4-methylphenyl)sulfonyl]sulfinimidoyl]di-3,1-propanediyl ester, rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 196867-85-3
CMF C49 H53 N5 O10 S2



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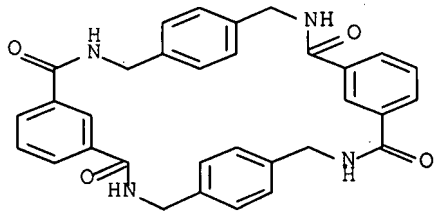

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FULL ESTIMATED COST	44.51	220.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.24	-6.24

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

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DICTIONARY FILE UPDATES: 27 AUG 2007 HIGHEST RN 945649-99-0

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http://www.cas.org/support/stngen/stndoc/properties.html

=> S 196867-86-4/RN

L7 1 196867-86-4/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

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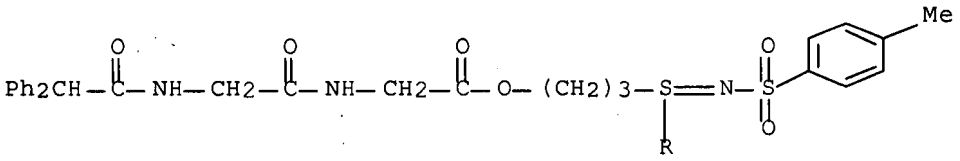
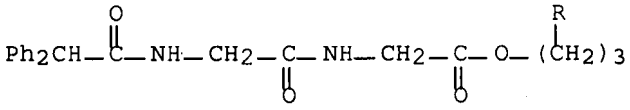
YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.55 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 196867-86-4 REGISTRY
CN Glycine, N-(diphenylacetyl)glycyl-, [[(4-methylphenyl)sulfonyl]sulfinimidoyl]di-3,1-propanediyl ester, rotaxane compd. with 3,11,18,26-tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3,11,18,26-Tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone, rotaxane compd. with N-(diphenylacetyl)glycylglycine [[(4-methylphenyl)sulfonyl]sulfinimidoyl]di-3,1-propanediyl ester (1:1) (9CI)
MF C49 H53 N5 O10 S2 . C32 H28 N4 O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); PRP (Properties)

CM 1

CRN 196867-85-3
CMF C49 H53 N5 O10 S2





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CRN 169203-75-2
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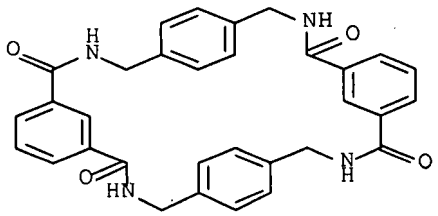

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

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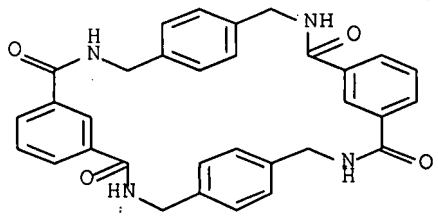
=> logoff hold

http://www.cas.org/support/stngen/stndoc/properties.html

=> s 169203-75-2
L1 1 169203-75-2
(169203-75-2/RN)

=> d scan

L1 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 3,11,18,26-Tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (9CI)
MF C32 H28 N4 O4
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

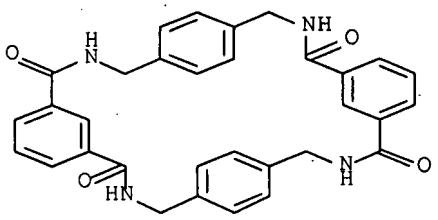
ALL ANSWERS HAVE BEEN SCANNED

ENTER DISPLAY FORMAT (IDE):all

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 169203-75-2 REGISTRY
ED Entered STN: 20 Oct 1995
CN 3,11,18,26-Tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1,7,14,20-Tetraaza-2,6,15,19-tetraoxo-3,5,9,12,16,18,22,25-tetrabenzocyclohexacosane
MF C32 H28 N4 O4
CI COM
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.NP Roles for non-specific derivatives from non-patents: RACT (Reactant or reagent)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6-C6-C6-C22N4	C6-C6-C6-C6-NC5NC6NC5NC6	6-6-6-6-26	C32N4	19506.4.5	1



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	11.64	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	11.73	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	11.74	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	11.74	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	11.74	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	11.74	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	11.74	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	11.74	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	11.74	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	11.74	pH 10 25 deg C	(1)
Boiling Point (BP)	1028.5+/-65.0 deg C	760 Torr	(1)
Density (DEN)	1.199+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	150.58+/-3.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	316.0+/-34.4 deg C		(1)
Freely Rotatable Bonds (FRB)	0		(1)
H acceptors (HAC)	8		(1)
H donors (HD)	4		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	12		(1)
Koc (KOC)	201.09	pH 1 25 deg C	(1)
Koc (KOC)	202.62	pH 2 25 deg C	(1)
Koc (KOC)	202.78	pH 3 25 deg C	(1)
Koc (KOC)	202.79	pH 4 25 deg C	(1)
Koc (KOC)	202.79	pH 5 25 deg C	(1)
Koc (KOC)	202.79	pH 6 25 deg C	(1)
Koc (KOC)	202.79	pH 7 25 deg C	(1)
Koc (KOC)	202.79	pH 8 25 deg C	(1)
Koc (KOC)	202.79	pH 9 25 deg C	(1)
Koc (KOC)	202.75	pH 10 25 deg C	(1)
LOGD (LOGD)	1.71	pH 1 25 deg C	(1)
LOGD (LOGD)	1.71	pH 2 25 deg C	(1)
LOGD (LOGD)	1.71	pH 3 25 deg C	(1)
LOGD (LOGD)	1.71	pH 4 25 deg C	(1)
LOGD (LOGD)	1.71	pH 5 25 deg C	(1)
LOGD (LOGD)	1.71	pH 6 25 deg C	(1)
LOGD (LOGD)	1.71	pH 7 25 deg C	(1)
LOGD (LOGD)	1.71	pH 8 25 deg C	(1)
LOGD (LOGD)	1.71	pH 9 25 deg C	(1)
LOGD (LOGD)	1.71	pH 10 25 deg C	(1)
LOGP (LOGP)	1.710+/-0.678	25 deg C	(1)
Mass Intrinsic Solubility	0.0038 g/L	25 deg C	(1)

(ISLB.MASS)			
Mass Solubility (SLB.MASS)	0.0038 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0038 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0038 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0038 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0038 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0038 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0038 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0038 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0038 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0038 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0038 g/L	Unbuffered Water pH 7.00 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.0000071 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0000071 mol/L	Unbuffered Water pH 7.00 25 deg C	(1)
Molar Volume (MVOL)	444.1+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	532.59		(1)
PKA (PKA)	13.10+/-0.20	Most Acidic 25 deg C	(1)
PKA (PKA)	-1.07+/-0.20	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	116.40 A**2		(1)
Vapor Pressure (VP)	0 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2007 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

41 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
41 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 145:404775 CA Full-text
TI Adsorption of Fumaramide [2]Rotaxane and Its Components on a Solid Substrate: A Coverage-Dependent Study
AU Whelan, Caroline M.; Gatti, Francesco; Leigh, David A.; Rapino, Stefania; Zerbetto, Francesco; Rudolf, Petra
CS Laboratoire Interdisciplinaire de Spectroscopie Electronique, Facultes Universitaires Notre-Dame de la Paix, Namur, B-5000, Belg.
SO Journal of Physical Chemistry B (2006), 110(34), 17076-17081
CODEN: JPCBFK; ISSN: 1520-6106
PB American Chemical Society

DT Journal
LA English
CC 66-3 (Surface Chemistry and Colloids)
AB The coverage-dependent adsorption on Au(111) of a fumaramide [2]rotaxane and its components, a benzylic amide macrocycle and a fumaramide thread, is studied using high-resolution electron energy loss spectroscopy (HREELS). Up to monolayer coverage, the relative intensity of out-of-plane to in-plane Ph ring vibrational modes indicates that the macrocycle adopts an orientation with the Ph rings largely parallel to the surface. The formation of a chemisorption bond is evidenced by the presence of a Au-O stretching vibration. In contrast, the thread shows no evidence of chemisorption or a preferential orientation. The introduction of the thread into the macrocycle partly disrupts the film order so that the resulting chemisorbed rotaxane shows intermediate behavior with a preferential orientation up to 0.5 ML coverage. A decrease in film order and the absence of a preferred mol. orientation is observed for all three mols. at multilayer coverages. The spectral differences are addressed by mol. dynamics simulations in terms of the mobility of the phenyls of the three mols. on Au(111).
ST adsorption fumaramide rotaxane component gold surface chemisorption
IT Chemisorption
Molecular orientation
(adsorption of fumaramide rotaxane and its component on gold surface)
IT 7440-57-5, Gold, processes
RL: CPS (Chemical process); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(adsorption of fumaramide rotaxane and its component on gold surface)
IT 169203-75-2 299433-82-2 299433-83-3
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(adsorption of fumaramide rotaxane and its component on gold surface)
RE.CNT 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS RECORD
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AN 145:15410 CA Full-text
TI Surface Enhanced Second Harmonic Generation from Macrocycle, Catenane, and Rotaxane Thin Films: Experiments and Theory
AU Arfaoui, Imad; Bermudez, Veronica; Bottari, Giovanni; De Nadai, Celine; Jalkanen, Jukka-Pekka; Kajzar, Francois; Leigh, David A.; Lubomska, Monika; Mendoza, Sandra M.; Niziol, Jacek; Rudolf, Petra; Zerbetto, Francesco
CS Materials Science Centre, University of Groningen, Groningen, NL-9747 AG, Neth.
SO Journal of Physical Chemistry B (2006), 110(15), 7648-7652
CODEN: JPCBFK; ISSN: 1520-6106
PB American Chemical Society
DT Journal
LA English
CC 66-3 (Surface Chemistry and Colloids)
AB Surface enhanced second harmonic generation (SE SHG) expts. on mol. structures, macrocycles, catenanes, and rotaxanes, deposited as monolayers and multilayers by vacuum sublimation on silver, are reported. The measurements show that the mols. form ordered thin films, where the highest degree of order is observed in the case of macrocycle monolayers and the lowest in the case of rotaxane multilayers. The second harmonic generation activity is interpreted in terms of elec. field induced second harmonic (EFISH) generation where the elec. field is created by the substrate silver atoms. The measured second order nonlinear optical susceptibility for a rotaxane thin film is compared with that obtained by considering only EFISH contribution to SHG intensity. The elec. field on the surface of a silver layer is calculated by using the Delphi4 program for structures obtained with TINKER mol. mechanics/dynamics simulations. An excellent agreement is observed between the calculated and the measured SHG susceptibilities.
ST surface enhanced second harmonic generation macrocycle catenane rotaxane film
IT Monolayers
Second-harmonic generation
(surface-enhanced second harmonic generation of macrocycle, catenane, and rotaxane film on silver)
IT 7440-22-4, Silver, uses
RL: NUU (Other use, unclassified); USES (Uses)
(surface-enhanced second harmonic generation of macrocycle, catenane, and rotaxane film on silver)
IT 169203-75-2 252266-63-0 299433-83-3
RL: PRP (Properties)
(surface-enhanced second harmonic generation of macrocycle, catenane, and rotaxane film on silver)
RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(14) Johnston, A; Angew Chem, Int Ed Engl 1995, V34, P1212 CAPLUS
(15) Johnston, A; J Am Chem Soc 1996, V118, P10662 CAPLUS
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REFERENCE 3

AN 144:179928 CA Full-text
TI Surface enhanced SHG from macrocycle, catenane and rotaxane thin films: experiments and theory
AU Arfaoui, Imad; Bermudez, Veronika; De Nadai, Celine; Jalkanen, Jukka-Pekka; Kajzar, Francois; Leigh, David; Lubomska, Monika; Mendoza, Sandra M.; Niziol, Jacek; Rudolf, Petra; Zerbetto, Francesco
CS Mater. Sci. Cent., Univ. of Groningen, Groningen, NL-9747, Neth.
SO Proceedings of SPIE-The International Society for Optical Engineering (2005), 5724(Organic Photonic Materials and Devices VII), 139-148
CODEN: PSISDG; ISSN: 0277-786X
PB SPIE-The International Society for Optical Engineering
DT Journal
LA English
CC 73-10 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
AB Surface enhanced second harmonic generation expts. on supramols.: macrocycles, catenanes and rotaxanes, monolayers and multilayers deposited by vacuum evaporation on silver layers are reported and described. The measurements show that the mols. are ordered in thin films. The highest order is observed in the case of macrocycles and the lowest in thin films of fumaramide [2] rotaxanes. Also a better ordering is observed in the case of monolayers. The observed second harmonic generation activity is interpreted in terms of elec. field induced second harmonic generation. The elec. field contributing to SHG signal is created by silver atoms on the surface of silver layers. The measured second order NLO susceptibilities for a fumaramide [2] rotaxane is compared with that obtained by considering only EFISH contribution to SHG intensities. The elec. filed on the surface of silver layer is calculated using TINKER mol. mechanics/dynamics software and the Embedded Atom model. An excellent agreement is observed between the calculated and the measured SHG susceptibilities.
ST macrocycle catenane rotaxane film surface enhanced SHG expt theory
IT Electric field effects
Nonlinear optical susceptibility
Polarization
(surface enhanced second harmonic generation from macrocycles, catenanes, rotaxanes, monolayers and multilayers deposited by vacuum evaporation on silver and gold layers)
IT Films
Second-harmonic generation
(surface enhanced second harmonic generation from macrocycles, catenanes, rotaxanes, monolayers and multilayers deposited by vacuum evaporation on silver layers)
IT 7440-57-5, Gold, uses

RL: NUU (Other use, unclassified); USES (Uses)
(surface enhanced second harmonic generation from macrocycles, catenanes, rotaxanes, monolayers and multilayers deposited by vacuum evaporation on silver and gold layers)

IT 7440-22-4, Silver, uses
RL: NUU (Other use, unclassified); USES (Uses)
(surface enhanced second harmonic generation from macrocycles, catenanes, rotaxanes, monolayers and multilayers deposited by vacuum evaporation on silver layers)

IT 169203-75-2 184017-69-4 184017-75-2
RL: PRP (Properties)
(surface enhanced second harmonic generation from macrocycles, catenanes, rotaxanes, monolayers and multilayers deposited by vacuum evaporation on silver layers)

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD

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(11) Johnston, A; Angew Chem Int Ed Engl 1995, V34, P1212 CAPLUS
(12) Johnston, A; J Am Chem Soc 1996, V118, P10662 CAPLUS
(13) Kundrot, C; J Comput Chem 1991, V12, P402 CAPLUS
(14) Lane, A; J Am Chem Soc 1997, V119, P11092 CAPLUS
(15) Ponder, J; J Comput Chem 1987, V8, P1016 CAPLUS
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(18) Whelan, M; J Phys Chem B 2002, V106, P8739

REFERENCE 4

AN 143:279363 CA Full-text
TI Antitumor agents containing an amide[2]catenane
IN Ono, Nobufumi
PA Japan
SO Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C07D257-10
ICS A61K031-395; A61P035-00
CC 1-6 (Pharmacology)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2005247790	A	20050915	JP 2004-63370	20040308
	JP 3741706	B2	20060201		
	WO 2005085215	A1	20050915	WO 2004-JP12392	20040827

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,

AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

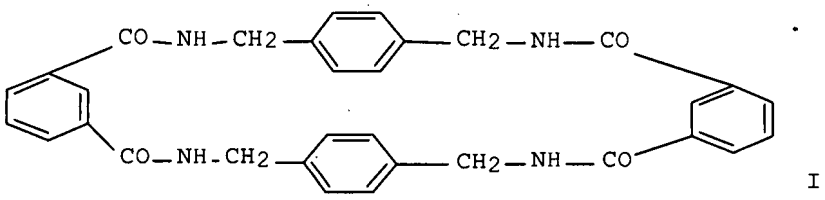
EP 1724265 A1 20061122 EP 2004-772348 20040827
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LI, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR

CN 1953966 A 20070425 CN 2004-80042350 20040827

PRAI JP 2004-63370 20040308

WO 2004-JP12392 20040827

GI



I

AB Antitumor agents, which are difficult to be effluxed from tumor cells, contain a self-catenane of 3,11,18,26-Tetraazapentacyclo[26.2.2.213,16.15,9.120,24]hexatriaconta-5,7,9(36),13,15,20,22,24(33),28,30,31,34-dodecaene-4,10,19,25-tetrone (I). Thus, a DMSO solution of I was electroporated to colon-26 cells to inhibit cell growth. I at 20 mg/kg p.o. showed slight toxicity on mice.

ST amide catenane antitumor electroporation

IT Antitumor agents
Electroporation
Neoplasm
(antitumor agents containing an amide[2]catenane which is slightly effluxed from tumor cells)

IT 169203-75-2
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(self-catenane; antitumor agents containing an amide[2]catenane which is slightly effluxed from tumor cells)

REFERENCE 5

AN 142:488084 CA Full-text

TI IRAS investigation of a catenane adsorption on Au(111)

AU Fustin, C. A.; Haq, S.; Wingen, A.; Gregoire, C.; Raval, R.; Dumas, P.; Hannam, J. S.; Leigh, D. A.; Rudolf, P.

CS Laboratoire Interdisciplinaire de Spectroscopie Electronique, Facultes Universitaires Notre Dame de la Paix, Namur, B-5000, Belg.

SO Surface Science (2005), 580(1-3), 57-62
CODEN: SUSCAS; ISSN: 0039-6028

PB Elsevier B.V.

DT Journal

LA English

CC 66-3 (Surface Chemistry and Colloids)

AB The adsorption of a benzylic amide [2]catenane on a Au(1 1 1) single crystal was studied using IR reflection absorption spectroscopy. The evolution of the IR spectra during catenane deposition at different temps. of the Au substrate (300 and 90 K) was compared. Evidence of the catenane deformation upon chemisorption were found at 300 K only. At 90 K the catenane is weakly adsorbed without any deformation.

ST catenane adsorption gold surface deformation state

IT Chemisorption
Deformation (mechanical)
Surface state
Surface structure
(catenane adsorption on Au(111))

IT 169203-75-2
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(catenane adsorption on Au(111))

IT 7440-57-5, Gold, properties
RL: PRP (Properties)
(catenane adsorption on Au(111))

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD

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REFERENCE 6

AN 142:463228 CA Full-text

TI Optical and low frequency electric field testing of the mobility of mobile parts in catenanes and rotaxanes

AU Nowicka, K.; Chollet, P. A.; Kajzar, F.; Bottari, G.; Gatti, F. G.; Leigh, D. A.; Miniewicz, A.

CS Commissariat a l'Energie Atomique DRT-LIST, DECS/SE2M/LCOF, CEA/Saclay, Gif sur Yvette, 91191, Fr.

SO Nonlinear Optics, Quantum Optics (2004), 32(1-3), 175-186
CODEN: NOQOAP; ISSN: 1543-0537

PB Old City Publishing, Inc.

DT Journal

LA English

CC 22-3 (Physical Organic Chemistry)

AB Optical and low frequency elec. fields are used to test the mobility of sub-parts of catenanes and rotaxanes in solution and in thin films. These mols. can be adequately tailored by the mol. engineering approach in order to enhance their response to external excitation. In particular the study of the Kerr electro-optic effect in solution permits testing of the rotational mobility of mols., or their parts, under the applied low frequency elec. field. Another possible movement can be created by illuminating the photoisomerizable rotaxane thread within its absorption band. This may lead to a "clipping" type movement made possible by the trans-cis isomerization process. The results of investigation of the influence of elec. optical and low frequency fields are presented and discussed in relation to the induced mobility of different parts of these complex mols.

ST mobility catenane rotaxane elec field

IT Isomerization
(cis-trans, photochem., of fumaramide/maleimide rotaxane; optical and low frequency elec. field testing of the mobility of mobile parts in catenanes and rotaxanes)

IT Isomerization
(cis-trans, thermal, of fumaramide/maleimide rotaxane; optical and low frequency elec. field testing of the mobility of mobile parts in catenanes and rotaxanes)

IT Electric field
(frequency and voltage dependence of Kerr effect; optical and low frequency elec. field testing of the mobility of mobile parts in catenanes and rotaxanes)

IT Kerr effect (electrooptical)
(in benzylic amide catenane; optical and low frequency elec. field testing of the mobility of mobile parts in catenanes and rotaxanes)

IT Molecular rotation
(of catenane; optical and low frequency elec. field testing of the mobility of mobile parts in catenanes and rotaxanes)

IT Catenanes
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(optical and low frequency elec. field testing of the mobility of mobile parts in catenanes and rotaxanes)

IT Rotaxanes
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(optical and low frequency elec. field testing of the mobility of mobile parts in catenanes and rotaxanes)

IT 509146-52-5
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(cis→trans thermal isomerization; optical and low frequency elec. field testing of the mobility of mobile parts in catenanes and rotaxanes)

IT 169203-75-2
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP

(Physical process); PROC (Process)
(self-catenane; Kerr effect; optical and low frequency elec. field testing of the mobility of mobile parts in catenanes and rotaxanes)

IT 299433-83-3
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(trans→cis photoisomerization; optical and low frequency elec. field testing of the mobility of mobile parts in catenanes and rotaxanes)

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(2) Bermudez, V; Mol Cryst Liq Cryst 2002, V374, P343 CAPLUS
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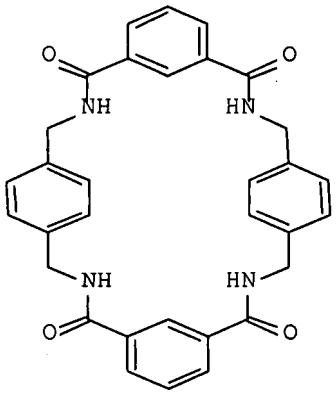
(21) Sauvage, J; Acc Chem Res 1998, V31, P611 CAPLUS

REFERENCE 7

AN 139:292240 CA Full-text
TI Clays as host matrix in the synthesis of organic macrocycles
AU Georgakilas, Vasilios; Gournis, Dimitrios; Bourlinos, Athanasios B.; Karakassides, Michael A.; Petridis, Dimitrios
CS Institute of Material Science, NCSR Demokritos Ag. Paraskevi Attikis, Athens, 15310, Greece
SO Chemistry--A European Journal (2003), 9(16), 3904-3908
CODEN: CEUJED; ISSN: 0947-6539
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))
GI



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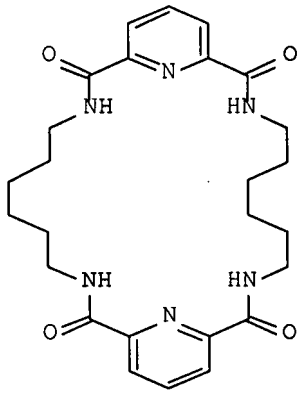

II

AB A new approach for the synthesis of amide macrocycles, based on the use of organo-clay derivs. as controlling template, is proposed as an alternative to the rotaxane method. Dications of p-xylylenediamine inserted in the clay interlayer space act as molding pillars around which neutral diamine mols. are erected via hydrogen bonding and π-π interactions to form supramol. arrays. Condensation of diamines in the supramol. arrays with diacid chlorides yields various tetramide macrocycles, e.g., I and II, in good yields. Shape, aromaticity and dimensions of the reactants are factors affecting the condensation reaction.

ST tetramide macrocycle prepn clay matrix; diacid chloride amidation clay matrix

IT Macrocyclic compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(clays as host matrix in preparation of tetramide macrocycles from diacid chlorides and diamines)

IT Cyclization
(lactamization; clays as host matrix in preparation of tetramide macrocycles
from diacid chlorides and diamines)

IT 99-63-8, Isophthaloyl chloride 124-09-4, 1,6-Hexanediamine, reactions 539-48-0, p-Xylylenediamine 2873-74-7, Glutaryl chloride 3057-45-2, 1,4-Benzenedimethanamine dihydrochloride 3739-94-4, 2,6-Pyridinedicarbonyl chloride 3857-36-1, 2,5-Thiophenedicarbonyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(clays as host matrix in preparation of tetramide macrocycles from diacid chlorides and diamines)

IT 169203-75-2P 169204-03-9P 169204-04-0P 423769-56-6P 607361-01-3P 607361-03-5P 607361-06-8P 607361-08-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(clays as host matrix in preparation of tetramide macrocycles from diacid chlorides and diamines)

IT 1318-93-0, Montmorillonite, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(sodium-rich; clays as host matrix in preparation of tetramide macrocycles from diacid chlorides and diamines)

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
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AN 137:359718 CA Full-text
TI Effect of potassium intercalation on the electronic and vibrational properties of benzylic amide [2]catenane films
AU Fustin, C. A.; Gouttebaron, R.; Caudano, R.; Rudolf, P.; Leigh, D. A.; Fanti, M.; Krug, A.; Zerbetto, F.
CS Laboratoire Interdisciplinaire de Spectroscopie Electronique, Facultes Universitaires Notre Dame de la Paix, Namur, B-5000, Belg.
SO Surface Science (2002), 515(1), 45-52
CODEN: SUSCAS; ISSN: 0039-6028
PB Elsevier Science B.V.
DT Journal
LA English
CC 73-6 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
AB The appearance of gap states in benzylic amide catenane thin films following K intercalation was studied by EELS and quantum chemical calcns. Both theory and experience find an excitation energy for transitions into these new states of .apprx.2 eV. The characteristics of these states are discussed.
ST intercalation vibration electronic transition potassium benzylic amide catenane
IT CNDO/S
Electronic structure
Intercalation
Molecular vibration
(effect of potassium intercalation on electronic and vibrational properties of benzylic amide [2]catenane films)
IT Electron energy loss spectroscopy
(high-resolution; effect of potassium intercalation on electronic and vibrational properties of benzylic amide [2]catenane films)
IT 7440-09-7, Potassium, properties
RL: MOA (Modifier or additive use); PRP (Properties); USES (Uses)
(effect of potassium intercalation on electronic and vibrational properties of benzylic amide [2]catenane films)

IT 169203-75-2
RL: PRP (Properties)
(effect of potassium intercalation on electronic and vibrational properties of benzylic amide [2]catenane films)

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REFERENCE 9

AN 137:253550 CA Full-text
TI Adsorption of a Benzylic Amide Macrocycle on a Solid Substrate: XPS and HREELS Characterization of Thin Films Grown on Au(111)
AU Whelan, Caroline M.; Cecchet, Francesca; Baxter, Richard; Zerbetto, Francesco; Clarkson, Guy J.; Leigh, David A.; Rudolf, Petra
CS Laboratoire Interdisciplinaire de Spectroscopie Electronique, Facultes Universitaires Notre-Dame de la Paix, Namur, B-5000, Belg.
SO Journal of Physical Chemistry B (2002), 106(34), 8739-8746
CODEN: JPCBFK; ISSN: 1520-6106
PB American Chemical Society
DT Journal
LA English
CC 66-3 (Surface Chemistry and Colloids)
AB Thin films of a benzylic amide macrocycle, the common component of a wide class of mech. interlocked mols., are prepared by vapor deposition on Au(111). The films are characterized by monochromated XPS and high resolution EELS (HREELS). The relative amts. of C, nitrogen, and oxygen are consistent with the formation of intact mol. species. At monolayer coverage, the relative intensity of out-of-plane to in-plane Ph ring vibrational modes indicates that the macrocycle adopts a nearly flat-lying conformation. The formation of a chemisorption bond is evidenced by the presence of a Au-O stretching vibration and a low binding energy component in the O 1s core level region assigned to interfacial bonding. A decrease in film order and the absence of a preferred mol. orientation is observed at higher coverages. Computer modeling of the adsorption of the macrocycle on the surface rationalizes the exptl. observations.

ST chemisorption film benzylic amide macrocycle gold XPS HREELS model

IT Configuration
(adsorbate; characterization of thin films of benzylic amide macrocycle adsorbed on Au(111) using XPS and HREELS)

IT Catenanes
Rotaxanes
RL: MSC (Miscellaneous)
(adsorption of benzylic amide macrocycle on Au(111) studied to make catenanes and rotaxanes technol. reality)

IT X-ray photoelectron spectra
(characterization of thin films of benzylic amide macrocycle adsorbed on Au(111) using XPS and HREELS)

IT Chemisorbed substances
(configuration; characterization of thin films of benzylic amide macrocycle adsorbed on Au(111) using XPS and HREELS)

IT Electron energy loss spectroscopy
(high-resolution, spectra; characterization of thin films of benzylic amide macrocycle adsorbed on Au(111) using XPS and HREELS)

IT Simulation and Modeling
(of adsorption of benzylic amide macrocycle on Au(111))

IT 7440-57-5, Gold, properties 169203-75-2
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(adsorption of benzylic amide macrocycle on Au(111) studied using XPS and HREELS)

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REFERENCE 10

AN 136:311628 CA Full-text
TI Organoclay derivatives in the synthesis of macrocycles
AU Georgakilas, Vasilios; Gournis, Dimitrios; Petridis, Dimitrios
CS Institute of Materials Science, NCSR "Demokritos" Ag., Athens, Greece
SO Angewandte Chemie, International Edition (2001), 40(22), 4286-4288
CODEN: ACIEF5; ISSN: 1433-7851
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 57
AB The tetraamide macrocycle was successfully synthesized from isophthaloyl dichloride and p-xylylenediamine using a sodium montmorillonite smectic clay as a template. The pillared clay was prepared from p-xylylenediamine dihydrochloride, neutral p-xylylenediamine was inserted into the pillared clay, the tetraamide macrocycle was formed by cyclocondensation of intercalated neutral p-xylylenediamine with isophthaloyl dichloride, and the product was extracted from clay.
ST tetraazatetraoxotetrabenzocyclohexacosane macrocycle synthesis
intercalated pillared montmorillonite clay cyclocondensation template
IT Clay minerals
RL: NUU (Other use, unclassified); USES (Uses)
(acidic, intercalated; organoclay derivs. as templates in the synthesis of macrocycles)
IT Macrocyclic compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(organoclay derivs. as templates in the synthesis of macrocycles)
IT Cyclocondensation reaction
(template; organoclay derivs. as templates in the synthesis of macrocycles)
IT 1318-93-0, Swy 1, uses
RL: NUU (Other use, unclassified); USES (Uses)
(organoclay derivs. as templates in the synthesis of macrocycles)
IT 3057-45-2
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process)
(organoclay derivs. as templates in the synthesis of macrocycles)
IT 99-63-8, Isophthaloyl dichloride 539-48-0, p-Xylylenediamine

RL: RCT (Reactant); RACT (Reactant or reagent)
(organoclay derivs. as templates in the synthesis of macrocycles)
IT 121-44-8, Triethylamine, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(organoclay derivs. as templates in the synthesis of macrocycles)
IT 169203-75-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(organoclay derivs. as templates in the synthesis of macrocycles)
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